OFFICE OF NAVAL RESEARCH

CONTRACT N00014-97-1-0066

R&T Code 33e 1806

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Technical Report No. 102

COMPUTED HEATS OF FORMATION

by

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April 9, 1998

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DTIC QUALITY INSPECTED 2

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

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i. Addito. God on a constant	April 9, 1998	Technical	5. FUNDING NUMBERS
4. TITLE AND SUBTITLE			
Computed Heats of Formation			N00014-97-1-0066
			Dr. Judah Goldwasser
5. AUTHOR(S)			R&T Code 33e 1806
	dward Grice, Monica C.	Concha and	
Pat Lane			
7. PERFORMING ORGANIZATION N.	AME(S) AND ADDRESS(ES)		8. PERFORMING ORGANIZATION REPORT NUMBER
University of New Orleans			
Department of Chemistry			102
New Orleans, Louisia	na 70148		
			10. SPONSORING / MONITORING
	ENCY NAME(S) AND ADDRESS(ES)		AGENCY REPORT NUMBER
Office of Naval Rese	arch		
Code 333			
800 N. Quincy Street Arlington, VA 22217			
11. SUPPLEMENTARY NOTES			
			TION CODE
12a. DISTRIBUTION / AVAILABILITY	STATEMENT		125. DISTRIBUTION CODE
	rologge		
Approved for public Unlimited distribution	ion.		
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13. ABSTRACT (Maximum 200 wor	Computed her	ats of formation fo	r 1 - 8.
NO ₂	NO_2 $Z Z$		
N N	Y	2. 72 II	NO
	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	3: Z = H $4: Z = NC$	O_2 O_2 N-N O_2
$N \rightarrow N$	$N \searrow N \longrightarrow $	5: Z = N	F_2 O_2N NO_2
NO ₂	0211	NO ₂	6
	NO ₂		o o
1	2		
	1: ΔH _f ^{298K} (s	solid) = 231 cal/g	5: ΔH_f^{298K} (solid) = 132 cal/g
O ₂ N	$ \begin{array}{c} 1: \Delta H_{f}^{298K} (s) \\ 2: \Delta H_{f}^{298K} (s) \\ 3: \Delta H_{f}^{298K} (s) \\ 4: \Delta H_{f}^{298K} (s) \end{array} $	solid) = 491 cal/g	6: ΔH_f^{298K} (solid) = 235 cal/g
$N-F$ K^+	NO ₂	-111 150 17	7: ΔH_f^{298K} (solid) = 1.5 cal/g
	3: ΔH _f ^{-3K} (solid) = 150 cal/g	$/: \Delta H_f$ (Solid) = 1.5 cal/g
7	4: ΔH_f^{298K} (s	solid) = 157 cal/g	О. ШТ
14. SUBJECT TERMS			15. NUMBER OF PAGES
Energetic compounds; heats of formation			16. PRICE CODE
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	THE STRUCTURE OF A CERTIFICATION	119. SECURITY CLASS	SECATION 20. LIMITATION OF ABSTRAC
17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	OF ABSTRACT	
Unclassified	Unclassified	Unclassifi	Standard Form 298 (Rev. 2-89)

We have computed heats of formation for compounds 1 - 8 (Table 1). The first five are target compounds proposed by M. Trudell (University of New Orleans); 6 - 8 have recently been prepared by R. Schmitt and J. Bottaro (SRI). For the molecular systems 1 - 7, we used our density functional procedure to obtain gas phase heats of formation, which were converted to liquid and solid state values by subtracting, respectively, the heats of vaporization and sublimation. The latter are determined by means of relationships that we have developed involving the computed electrostatic potential on the molecular surface [2,3]. (Vibrational energies were obtained from the molecular stoichiometries [4].) For the ionic solid 8, the heat of formation was calculated using the lattice enthalpy and the gas phase heats of formation of the positive and negative ions; the lattice enthalpy was computed from our recently-developed relationship involving anionic surface electrostatic potentials [5]. For comparison, the experimental solid phase heats of formation of HMX and RDX are, respectively, 60.4 cal/g and 76.1 cal/g [6].

References:

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 $\begin{array}{c} 1 \\ \\ O \\ \\ N \end{array} \begin{array}{c} NO_2 \\ \\ \\ NO_2 \end{array}$

$$\begin{split} \Delta H_f^{298K}\left(gas\right) &= 73.6 \text{ kcal/mole} = 341 \text{ cal/g} \\ \Delta H_f^{298K}\left(\text{liquid}\right) &= 60.0 \text{ kcal/mole} = 278 \text{ cal/g} \\ \Delta H_f^{298K}\left(\text{solid}\right) &= 49.8 \text{ kcal/mole} = 231 \text{ cal/g} \end{split}$$

$$\begin{split} \Delta H_f^{298K} \left(gas \right) &= 155 \text{ kcal/mole} = 604 \text{ cal/g} \\ \Delta H_f^{298K} \left(\text{liquid} \right) &= 139 \text{ kcal/mole} = 544 \text{ cal/g} \\ \Delta H_f^{298K} \left(\text{solid} \right) &= 126 \text{ kcal/mole} = 491 \text{ cal/g} \end{split}$$

$$\begin{split} \Delta H_f^{298K} & (gas) = 80.6 \text{ kcal/mole} = 263 \text{ cal/g} \\ \Delta H_f^{298K} & (liquid) = 64.3 \text{ kcal/mole} = 210 \text{ cal/g} \\ \Delta H_f^{298K} & (solid) = 45.8 \text{ kcal/mole} = 150 \text{ cal/g} \end{split}$$

4
$$O_2N NO_2$$
 $O_2N NO_2$ $O_2N NO_2$ $O_2N NO_2$ $O_2N NO_2$ $O_2N NO_2$

$$\begin{split} \Delta H_f^{298K}\left(gas\right) &= 104 \text{ kcal/mole} = 264 \text{ cal/g} \\ \Delta H_f^{298K}\left(\text{liquid}\right) &= 87.5 \text{ kcal/mole} = 221 \text{ cal/g} \\ \Delta H_f^{298K}\left(\text{solid}\right) &= 62.2 \text{ kcal/mole} = 157 \text{ cal/g} \end{split}$$

$$\begin{split} \Delta H_f^{298K} \left(gas \right) &= 96.5 \text{ kcal/mole} = 236 \text{ cal/g} \\ \Delta H_f^{298K} \left(\text{liquid} \right) &= 79.1 \text{ kcal/mole} = 194 \text{ cal/g} \\ \Delta H_f^{298K} \left(\text{solid} \right) &= 54.0 \text{ kcal/mole} = 132 \text{ cal/g} \end{split}$$

$$\Delta H_f^{298K} (gas) = 108 \text{ kcal/mole} = 370 \text{ cal/g}$$

$$\Delta H_f^{298K} (liquid) = 91.1 \text{ kcal/mole} = 312 \text{ cal/g}$$

$$\Delta H_f^{298K} (solid) = 68.7 \text{ kcal/mole} = 235 \text{ cal/g}$$

(continued)

Table 1. Computed heats of formation (continued).

7
$$O_2N$$
 $N-F$

$$\Delta H_f^{298K}$$
 (solid) = -69.0 kcal/mole = -584 cal/g

 ΔH_f^{298K} (gas) = 20.5 kcal/mole = 124 cal/g

 ΔH_f^{298K} (liquid) = 8.23 kcal/mole = 49.8 cal/g

 ΔH_f^{298K} (solid) = 0.24 kcal/mole = 1.5 cal/g

$$\mathbf{8} \qquad \qquad \mathbf{K}^{+} \left[\begin{array}{c} \mathbf{N} \overset{\mathbf{F}}{\searrow} \\ \mathbf{NO}_{2} \end{array} \right]^{-}$$